

### Supplementary material

**Table S1. Retention times and molecular masses of purified standard substances used in GC-MS for metabolite identification**

Derivatization of substances (MEOX) may lead to different retention times and molecular masses of fragments. Most standard substances were purchased from Sigma (Munich, Germany)

Retention time (min)	Substance name	Molecular mass
07,68	Pyruvate	174
08,94	Alanine	116
10,74	$\beta$ -Amino butyric acid	130
11,91	$\alpha$ -Ketocaproate	110
11,91	Valine	144
12,54	Urea	189
13,24	Ethanolamine	174
13,42	Leucine	158
14,00	Isoleucine	158
14,04	Proline	142
14,27	Maleic acid	245
14,30	Glycine	174
14,47	Succinate	247,409
14,69	Norleucine	158
15,09	Glycerate	189,192
15,18	Uracil	255,241
15,31	Fumarate	245
15,85	Serine	204
16,54	Threonine	101
16,82	Thymine	255
17,32	S-Methylcystein	218
17,40	$\beta$ -Alanine	248
17,96	Orcinol	253,268
18,08	Homoserine	218
18,63	Glutamine	155
19,11	Malate	245,307
19,72	Methionine	176
19,86	L-Aspartate	100,188,232
19,94	$\gamma$ -Amino butyric acid (GABA)	174,304

19,94	Hydroxyproline	230
20,00	Cytosine	240,257
20,23	Cinnamic acid/trans-Cinnamic acid	131,161,205
20,62	Cysteine	220
21,14	$\alpha$ -Hydroxyglutarate	203,247
21,15	$\alpha$ -Ketoglutarate	198
21,19	2-Isopropylmalate	275
21,81	Phosphoenolpyruvate (PEP)	369
21,96/22,47	Asparagine (4TMS)	216
22,00	Ornithine_Citrulline_Argenine_3TMS	216,348
22,13	Glutamate	230,246
22,24	Phenylalanine	192
23,07/23,30	Xylose	217,307
23,09	Homocysteine	128,234
23,41	Asparagine (3TMS)	231
23,44	Arabinose	217,307
23,78	Ribose	217
24,29	2-Amino adipate	260
24,60/24,72	Rhamnose	277
24,78	Ribitol	217
24,99	cis-Aconitate	229
25,10/25,35	Dihydro aceton phosphate (DHAP)	400
25,51	$\alpha$ -Glycero-P, Glycerol-3-P	357
25,52	N-Acetyl glutamine acid/N-Acetylglucosamine	156,274
25,94	Glycerate-2-P	299,315,459
26,18	Syringaldehyde	253,283
26,23	1-Methyl-L-histidine (TMS)	196
26,40	Shikimate	204
26,45	Citrulline_Ornithine_Argenine_4TMS	142
26,51	Glycerate-3-P	277,299,459
26,58	Arginine	157,256
26,68	Citrate	257
26,74	Isocitrate	245,319
27,04	Pinitole	260
27,05/27,19	2-Methylcitrate	287
27,42	Adenine	264
27,92/28,13	Fructose	307
28,08	Gluconolactone	129,220
28,30/28,71	Galactose	319
28,43/28,76	Glucose	319
28,51	Lysine	156
28,57	Histidine	154
28,71	Erythrose-4-P	357
28,79	p-Cumaric acid	219,249,293,308
28,85	Koniferyl aldehyde	217,218,248,278,279
28,90	Tyrosine	218

29,04	dihydro-Caffeic acid	179,398
29,17	Mannitol	217,319
29,19/29,48	Glucuronic acid	333
29,40/30,34	trans-Chalcone	206,236
29,98	Pantothenic acid	201
30,44	Gluconate	333
31,44	3-Hydroxy-4-methoxy-cinnamonic acid	249,293,308,323,338
31,76	Ferulic acid	249,293,308,323,338
31,92	trans-3,5-dimethoxy-4-hydroxy-cinnamonic acid/Sinapinic aldehyde	174,248
32,01	myo-Inositole	305
32,53	Ribose-5-P	299,315
32,56	Caffeic acid	219,381,396
32,60	Ribulose-5-P	357
33,99	L-Cystathionine_4TMS	128,218,245
34,07	Tryptophane	202
34,44	Sinapinic acid	323,338,368
34,63	Spermidine	201
35,42	Cystine	266,218
36,04	Fructose-6-P	315
36,24/36,52	Glucose-6-P	387
37,70	myo-Inositole-P	318
37,94	Gluconate-6-P	333,387
40,83	Adenosine	236
41,29	Saccharose	361
42,30	Cellobiose	361
42,76	Trehalose	361
42,77	Maltose	480
44,61/44,99	Melibiose	204,361
46,89	Coumesterole	412
48,42	Quercetine	647
49,42	Luteoline	559